Potential of Diffuse Reflectance Infrared Fourier Transform Spectroscopy and Chemometrics for Coffee Quality Evaluation

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***Abstract*—Given the successful application of spectroscopic methods in the field of coffee analysis as fast and reliable routine techniques, the objective of this work was to evaluate the feasibility of employing Diffuse Reflectance Infrared Fourier Transform Spectroscopy (DRIFTS) for discrimination between roasted coffees that presented distinct sensory characteristics and were submitted to a range of roasting conditions. Samples consisted of coffees obtained from Nespresso® type capsules of intensity levels ranging from 2 to 12. Principal Component Analysis (PCA) of the processed spectra provided separation of the samples into three groups: low (positive PC1), medium (scattered) and high (negative PC1) intensity. Group separation was related to both roasting intensity and sensory parameters, with a clear separation between samples described as low roasted with fruity and floral flavors in comparison to samples described as being intense and very roasted. PLS-DA models were constructed and provided satisfactory discrimination according to sensory characteristics. Samples were classified according to flavor as sugar browning, enzymatic, or dry distillation. Such results confirm the potential of DRIFTS in the discrimination and classification of roasted and ground coffees.**

***Index Terms*—chemometrics, coffee, DRIFTS, FTIR, spectroscopic methods**

I. Introduction

Over the last decades, the need for new and rapid analytical methods in the field of food analysis has prompted extensive research on spectroscopic methods, including Near Infrared Spectroscopy (NIRS) and Fourier Transform Infrared (FTIR) spectroscopy [1], [2]. Recent applications of such methods to coffee quality analysis include discrimination between Arabica and Robusta species [3], discrimination between defective and non-defective beans [4], [5] and discrimination between pure and adulterated coffee samples [6]-[9].

Spectroscopic methods are usually based on transmittance or reflectance readings, with reflectance-based methods being more commonly employed as routine methodologies for food analysis, since they require none or very little sample pre-treatment [10]. FTIR reflectance methods can be divided into Attenuated Total Reflectance Fourier Transform Infrared Spectroscopy (ATR-FTIR) and Diffuse Reflectance Fourier Transform Infrared Spectroscopy (DRIFTS). ATR collects information from the sample surface while DRIFTS provides information from the entire sample, being a combination of internal and external reflection [10]. Our previous studies have shown the feasibility of employing DRIFTS for detection of defective (low quality) coffee beans in admixtures with non-defective (high quality) ones [11] and also for detection and quantification of multiple adulterants in roasted and ground coffee [7]-[9]. In this study we extend our research by further evaluating the potential of this technique for discrimination between roasted coffees that presented distinct sensory characteristics under distinct roasting conditions.

II. Materials and Methods

A. Materials

Samples consisted of ground and roasted coffees obtained from Nespresso® type capsules of different brands and origins, with varying intensity levels and sensory characteristics, as specified in Table I.

B. Color Evaluation

All samples were further ground (0.15<D<0.5mm) and submitted to color evaluation. Color measurements were performed using a tristimulus colorimeter (HunterLab Colorflex 45/0 Spectrophotometer, Hunter Laboratories, VA, USA) with standard illumination D_{65} and colorimetric normal observer angle of 10°. Measurements were based on the CIE $L^*a^*b^*$ three dimensional cartesian (*xyz*) color space represented by: Luminosity (L^*), ranging from 0 (black) to 100 (white) - z axis; parameter a^*, representing the green-red color component - x axis; and parameter b^*, representing the blue-yellow component - y axis. Discussion of color results will only take into account the luminosity parameter, given that previous studies on coffee analysis have established that this is the most relevant parameter for color evaluation [9], [12].

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TABLE I. CLASSIFICATION OF COFFEE SAMPLES ACCORDING TO INTENSITY, SPECIES, AND SENSORY ATTRIBUTES SPECIFIED BY THE MANUFACTURERS

Sample	Intensity	Species	Sensory characteristics
Brand 1			
S1	9	Arabica	Cocoa, intense
S2*	9	Arabica	Cocoa, intense
S3	3	Arabica	Floral, intense
S4	5	Arabica, Robusta	Cereals, balanced
S5	3	Arabica	Fruity, citric
S6*	2	INP	INP
S7*	7	Arabica, Robusta	Cereals, roasted cocoa, high intensity
S8*	3	INP	INP
S9	11	Arabica	Intense, bitter cocoa notes
S10	4	Arabica	Sweet, cereals, balanced
S11	8	Arabica	Sweet cereal, roasted intense
S12	10	Arabica, Robusta	Spicy, intense
S13	12	Arabica, Robusta	Woody, intense, spicy
S14	4	Arabica	Malted cereal, balanced
S15	6	Arabica	Caramel aromas, balanced
S16	10	Arabica, Robusta	Soft, fruity, dark roast, intense
S17	8	Arabica, Robusta	Woody, intense
S18	6	Arabica	Fruity
S19	4	Arabica	Floral, fruity
S20*	4	Arabica	Floral, fruity
S21	4	Arabica	Fruity cereal, balanced
S22*	4	Arabica	Fruity cereal, balanced
Brand 2			
S23	INP	Arabica	Sweet and velvety coffee with balanced acidity and chocolate aromas
S24	INP	Arabica	Fragrant aroma and balanced flavor
Brand 3			
S25	4	Arabica	Soft and elegant aroma
S26	5	Arabica	Balanced and aromatic blend of beans from the highlands
S27	10	Arabica	Delicate aromas of roasting
S28	5	Arabica	Walnuts
S29	9	Arabica	Cocoa aroma and Strong body flavor
S30	4	Arabica	Fruity notes and balanced acidity
Brand 4			
S31	INP	Arabica	Citric notes
S32	INP	Arabica	Fruity aroma and mild acidity
S33	INP	Arabica	Caramelized and fruity notes, well balanced coffee
Brand 5			
S34	10	Arabica	Dark chocolate notes and toasted hazelnuts
S35	7	Arabica	Nuts, citric

*Decaffeinated coffee.
INP: Information not provided.

C. FTIR Analysis

A Shimadzu IRAffinity-1 FTIR Spectrophotometer (Shimadzu, Japan) with a DLATGS (Deuterated Triglycine Sulfate Doped with L-Alanine) detector was used in the measurements that were all performed in a dry atmosphere at room temperature (20±0.5 °C). Diffuse Reflectance (DR) measurements were performed with a Shimadzu sampling accessory (DRS8000A). Each sample was mixed with KBr and 23mg of this mixture were placed inside the sample port. Pure KBr was employed as reference material (background spectrum). All spectra were recorded within a range of 4000-600cm^{-1} with a 4cm^{-1} resolution and 20 scans.

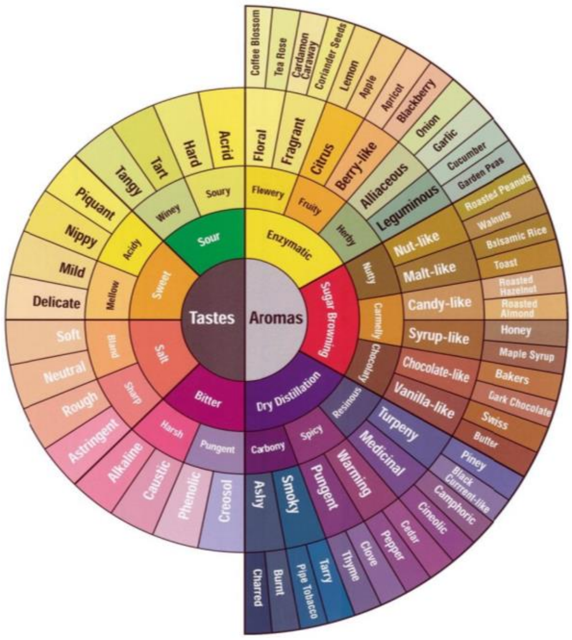


Figure 1. SCAA flavor wheel for sensory classification of roasted coffees (SCAA, 2015).

TABLE II. CLASSIFICATION OF COFFEE SAMPLES ACCORDING TO INTENSITY, SPECIES, AND SENSORY ATTRIBUTES SPECIFIED BY THE MANUFACTURERS

Class	Sensory characteristics	Samples
Sugar Browning	Cocoa, cereals, roasted cocoa, bitter cocoa, sweet, cereals malted cereal, caramel aromas, dark roast, chocolate aromas, walnuts, aromas of roasting, cocoa aroma, strong body flavor, caramelized notes, dark chocolate notes, toasted hazelnuts	S1, S2*, S4, S7*, S9, S10, S11, S14, S15, S27, S28, S29, S34
Enzymatic	Floral, fruity, citric, acidity, mild acidity, fruity aroma, fruity notes	S3, S5, S18, S19, S20*, S24, S30, S31, S32
Dry Distillation	Woody, spicy	S13, S17
Uncategorized	Soft and elegant aroma, balanced and aromatic blend of beans from the highlands; delicate aromas of roasting	S25, S26, S27
Combination of attributes	Sweet, cereals, balanced; soft, fruity, dark roast, intense; sweet and velvety coffee with balanced acidity and chocolate aromas; caramelized and fruity notes, well balanced coffee; nuts, citric	S16, S21, S22*, S23, S33, S35

*Decaffeinated coffee.

D. Data Processing and Statistical Analysis

In order to reduce the effect of noise, remove redundant information and enhance sample-to-sample differences, the following data pre-processing (pretreatment) techniques were applied to the obtained spectra: mean centering, Generalized Least Squares Weighting (GLSW), for PCA analysis, and Orthogonal Signal Correction (OSC), for PLS-DA analysis. Samples were classified as: low (intensity≤4), medium (5≤intensity≤8) or high (intensity≥9) intensity. SCAA (Specialty Coffee Association of America) classification was employed for separation of the samples into groups according to sensory attributes as shown in Fig. 1 [13]. Samples were classified into major groups as shown in Table II. The statistical packages MATLAB 7.13 (The MathWorks, Natick, Massachusetts, EUA) and PLS Toolbox (Eigenvector Technologies, Manson, Washington) were employed for the chemometric calculations.

III. Results and Discussion

Color measurements results (average luminosity values) are displayed in Table III. It can be noticed that, in general, the samples classified with higher intensity presented the lowest luminosity value whereas the low intensity samples presented the highest luminosity values. Such results indicate that intensity is probably related to roasting degree, although roasting conditions were not specified by the manufacturers. However, variance analysis results (One-way ANOVA) indicated that there was no significant difference among samples (see Table IV). Therefore, luminosity is not an isolated factor and cannot be directly correlated to intensity values. Such results are in agreement with the data from Dmowski and Dabrowska [14], who reported that there was not a strong correlation between luminosity and roasting intensity.

TABLE III. Average Luminosity Values

Intensity Classes	Intensity value	Luminosity (L*) Standard deviation
High Intensity	9 a 12	19.28 ±1.64
Medium Intensity	5 a 8	19.64 ±2.0
Low Intensity	2 a 4	20.68 ±2.8

TABLE IV. One-Way Analysis of Variance for Luminosity Values

Source	Sum of squares	Degrees of freedom	Mean squares	F
Between groups of intensity	25.29415335	2	12.64707668	2.251376729
Inside groups of intensity	179.7595438	32	5.617485743	
Total	205.0536971	34		

F value=3.2945; p-value=0.12; α=0.05

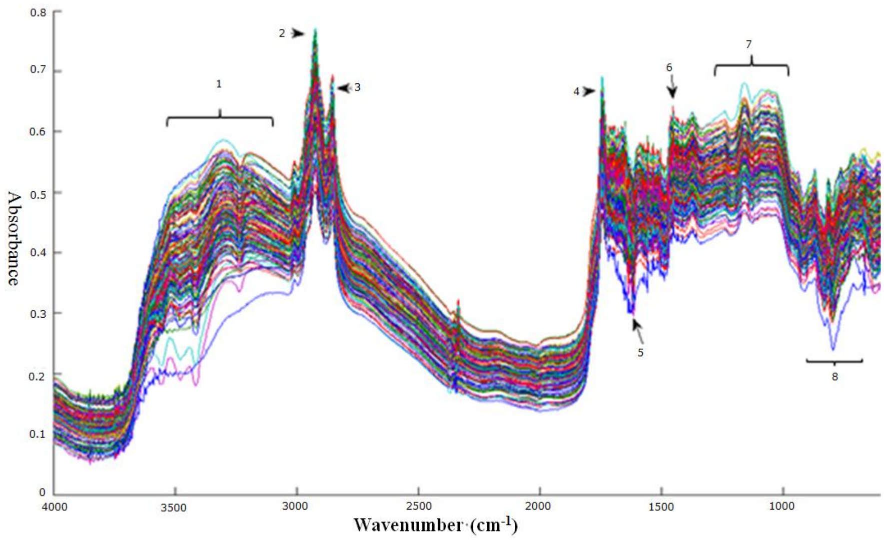


Figure 2. Diffuse reflectance spectra obtained for roasted coffees from espresso capsules.

Typical average spectra obtained for the evaluated samples are shown in Fig. 2. The large band at 3700-3000cm^{-1} (band 1) is attributed to O-H stretching and it is usually associated to residual moisture in the samples [15]. Bands 2 and 3 have been previously identified in spectra of roasted and crude coffee samples and also in spectra of caffeinated beverages [7], [16]. They can be partly assigned to unsaturated and saturated lipids present in coffee. Band 3 has also been attributed to stretching of C-H bonds of methyl ($–CH_3$) group in the caffeine molecule and employed in predictive models for quantitative analysis of caffeine [16]. Band 4 is attributed to C=O stretching in lipids [15]. Absorption in region 5 can be associated to several substances that are commonly found in roasted coffee, including caffeine, trigonelline and pyridines. Band 6 is attributed to C-H vibrations from glicerol. Region 7 is called "fingerprint region" and is characterized by vibrations of several types of bonds, including C-H, C-O and C-N, in association to carbohydrates [17]. The several bands in region 8 can be attributed to β-glycosidic links from coffee carbohydrates (e.g., arabinogalactans, galactomannans and cellulose) and also chlorogenic acids.

Using the DR spectra as chemical descriptors, Principal Component Analysis (PCA) was applied in order to establish whether samples could be separated.

Data matrices were constructed so that each row corresponded to a sample and each column represented the spectra datum at a given wavenumber, after processing as previously described. Results are displayed in Fig. 3. The first component accounted for 11% of the total sample variance. It can be seen that the high intensity samples (negative PC1) are well separated from the low intensity ones (positive PC1). An analysis of the loadings plots (Fig. 4) associates positive PC1 with carbohydrates, chlorogenic and carboxilic acids (1700, 1574 and 1073cm^{-1}) and negative PC1 with caffeine, lipids and carbohydrates (2920, 1740 and 791cm^{-1}). Results indicate that not only roasting intensity but also flavor components might be affecting sample grouping.

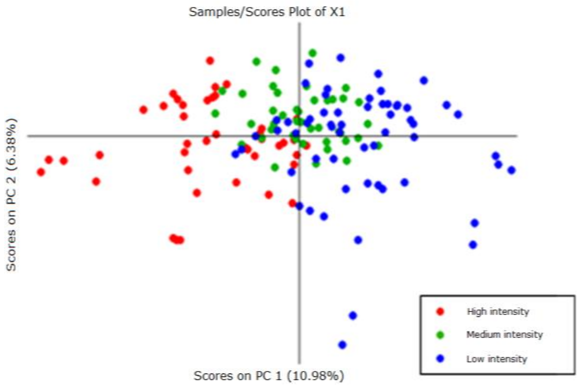


Figure 3. PCA score plots (PC1 vs. PC2) of the spectra submitted to mean centering and GLSW.

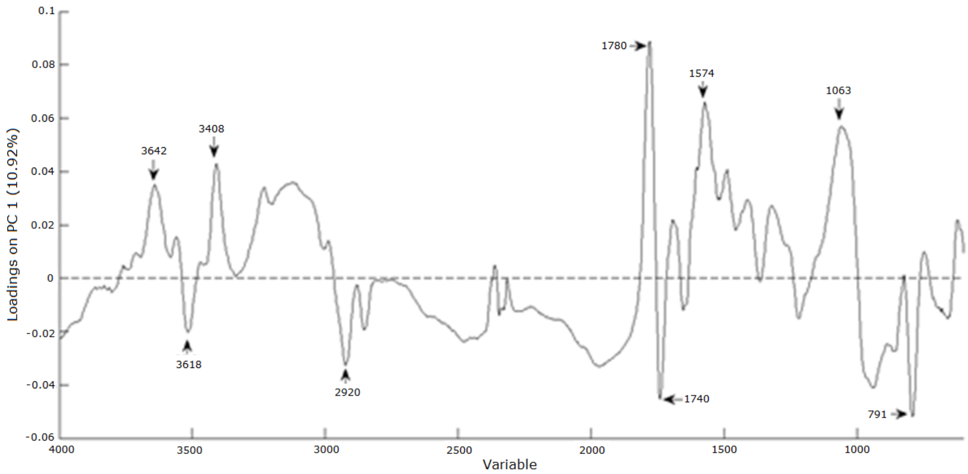


Figure 4. PC1 loading plot of the spectra submitted to mean centering and GLSW.

Results from PCA analysis of decaffeinated vs. regular samples are shown in Fig. 5. The first component accounted for 15.5% of the total sample variance. A clear separation between decaffeinated (negative PC1) and regular (positive PC1) samples can be seen. An analysis of the loadings plots (not shown) associates positive PC1 with the bands at 1699 and 1653cm^{-1}, characteristic of caffeine as well as trigonelline.

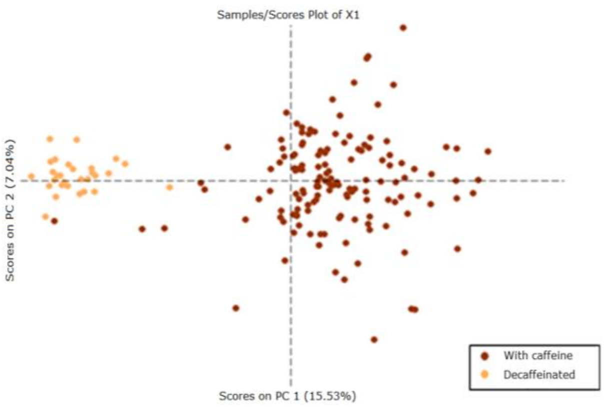


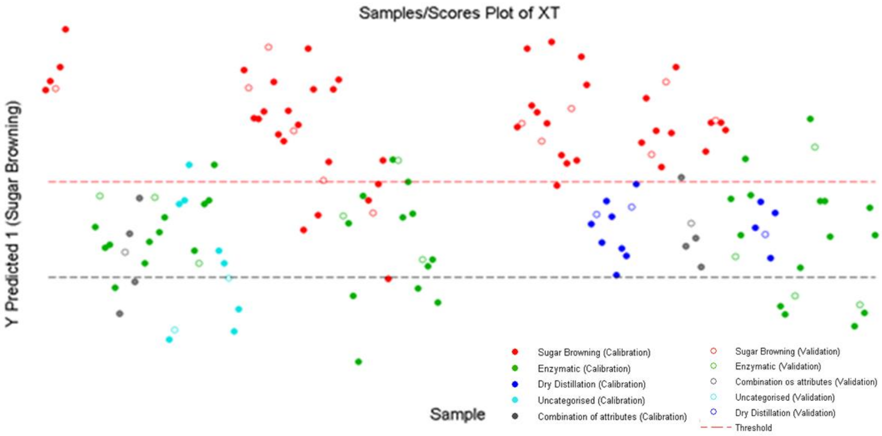
Figure 5. PCA score plots (PC1 vs. PC2) of the spectra submitted to mean centering and GLSW.

PLS-DA models were constructed by using the data obtained the regular coffee samples, i.e., decaffeinated samples were excluded. The calibration and validation sets consisted of a total of 103 and 43 samples, respectively. The best discrimination model was constructed with 17 latent variables, and accounted for 99.8% and 62.7% of the variance in *X* (spectral data) and *Y* (sensory classification), respectively. The sensitivity (percent of true positives) and specificity (percentage of true negatives) parameters are shown in Table V. Sensitivity and specificity values obtained for both calibration and validation samples are high, confirming the accuracy of the developed models.

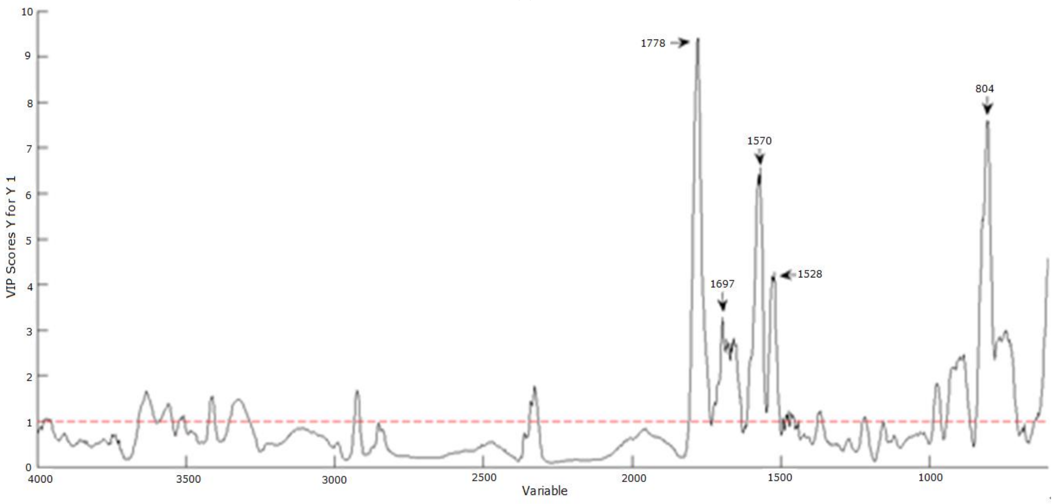
TABLE V. SENSITIVITY AND SPECIFICITY VALUES FOR THE TRAINING (CALIBRATION) AND TESTING (VALIDATION) SETS

	Sugar Browning	**Enzymatic**	**Dry Distillation**	**Combination of attributes**
Calibration Set				
Sensitivity	0.87	0.825	1	1
Specificity	0.897	0.865	0.980	1
Validation Set				
Sensitivity	0.826	0.700	0.750	1
Specificity	0.838	0.730	0.75	0.943
Cross Validation Classification Error	**0.17**	**0.28**	**0.15**	**0.02**

Predicted Y values for the “Sugar Browing” model are shown in Fig. 6(a) and the corresponding variable importance in projection (VIP) scores are shown in Fig. 6(b). VIP scores estimate the importance of each variable in the projection used in a PLS-DA model and are commonly used for variable selection. Variables with a large VIP score can be considered important in given model, whereas variables presenting VIP scores significantly smaller than 1 (one) are less important and might be good candidates for exclusion from the model. The most important bands (variables) for discrimination of coffees within this sensory class were 1778, 1690, 1570, 1508 and 804 cm^{-1} and can be associated to lipids, caffeine, trigonelline and carbohydrates.



(a)



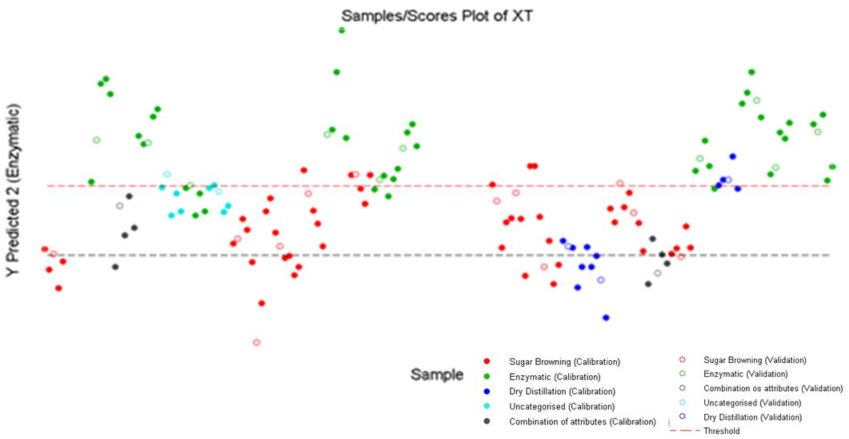
(b)

Figure 6. “Sugar Browning” PLSDA model of the spectra submitted to mean centering and OSC: (a) predicted Y values and (b) VIP scores.

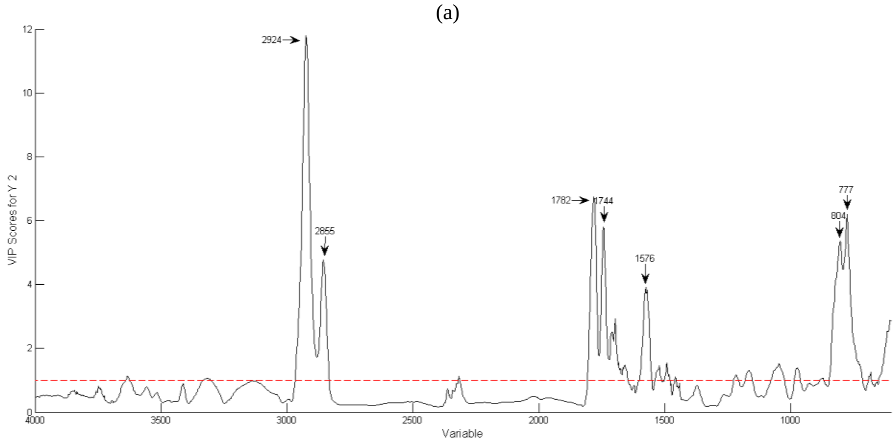
Aroma groups such as almonds, nuts, cocoa and sweetness are consistent in lighter and medium roasts [18]. The coffee tasters notice these descriptors, especially chocolate, when the beans are subjected to medium-dark roasts. An additional minute at the grain heating phase during roasting can contribute to increased sweetness and a greater concentration of aldehydes and acids that are related to chocolate and nut flavorings [19].

Carbohydrates have a significant impact on the sweetness of the beverage and the caramel notes from the Maillard reactions occurring between sugars and amino acids during roasting. The lipid fraction retains important volatile flavor compounds as well as contributes to its tactility, commonly known as the “body” of the drink [20]. The trigonelline molecules are responsible for the organoleptic characteristics of the beverage and are related to roasted coffee aroma [21]-[22]. Thus, the molecules that contribute to the classification of the model samples are directly related to the aromatic compounds of the caramelization of the sugars. Almond aromas are more noticeable in lighter roasts and cocoa aromas in medium roasts [18].

Predicted Y values for the “Enzimatic” model are shown in Fig. 7(a) and the corresponding VIP scores are shown in Fig. 7(b). The most important bands that provided discrimination of this specific class were 2922, 2851, 1780, 1742, 1570, 775 and 772cm^{-1}. These regions are related to lipids, caffeine, carbonyl, aliphatic acids and esters, trigonelline and carbohydrates. Floral, fruity, herbal and citrus aromas are typically assigned to this sensory class. Floral aromas are commonly exhibited by esters and acids, depending on the type and concentration of carbonyl in the roasted coffee, which significantly contributes to the flavor [19]. Trigonelline may have contributed to the separation of samples for this class along with the lipid fraction [20] as discussed earlier.

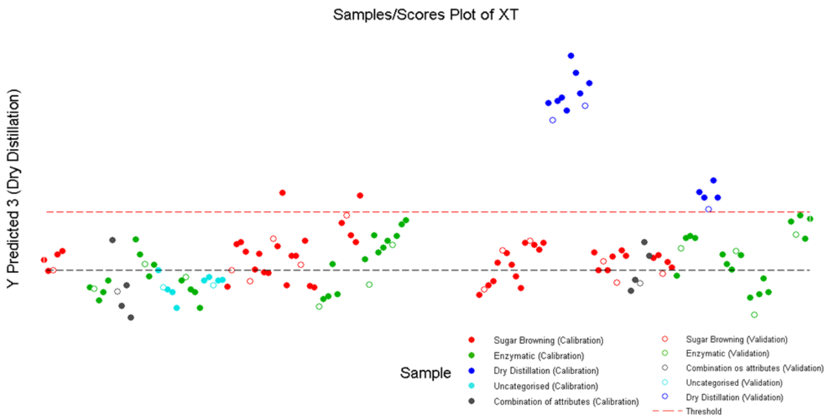


(a)

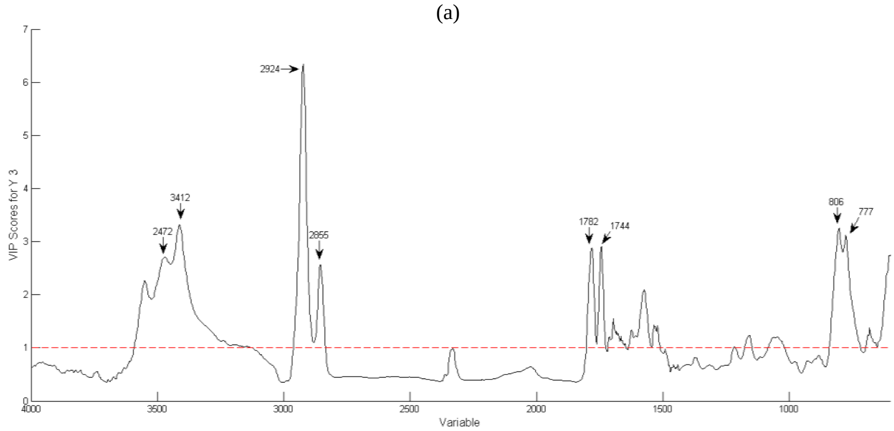


(b)

Figure 7. "Enzymatic" PLSDA model of the spectra submitted to mean centering and OSC: (a) predicted Y values and (b) VIP scores.



(a)



(b)

Figure 8. "Dry Distillation" PLSDA model of the spectra submitted to mean centering and OSC: (a) predicted Y values and (b) VIP scores.

Results regarding the "Dry Distillation" model are shown in Fig. 8. The VIP score data indicate that the regions and bands that contributed the most for discrimination of these samples were: 3550-3400, 2922, 2851, 1778-1741, 1570 and 775-773cm^{-1}. These can be associated to the presence of lipids, caffeine, carbonyl, aliphatic acids, and carbohydrates. The set of attributes that characterize this sensory class are related to pungency, and woody, charred and spicy aromas. According the literature, aliphatic acids are correlated to wood and cucumber aromas [19]. The lipids may have contributed by retaining important volatile compounds, as previously described. The carbohydrates are assigned as responsible for sweetness and production of other aromatic compounds by the Maillard reaction [20]. Many sensory attributes related to "Dry Distillation", such as smokey, burnt and pungent, are perceived more intensely with increased degree of roasting [18].

IV. Conclusions

Diffuse Reflectance Infrared Fourier Transform Spectroscopy together with chemometric techniques was successfully employed for discrimination between roasted coffees that presented distinct sensory characteristics. PCA analysis provided separation according to roasting intensity and also between regular and decaffeinated samples. Separation was affected by roasting intensity and sensory parameters, with a clear separation between samples described as low roasted with fruity and floral flavors in comparison to samples described as being very intense and very roasted. PLS-DA models were constructed and provided satisfactory discrimination according to sensory characteristics. SCAA based classification provided separation of the samples mainly as "Sugar browning", "Enzymatic" or "Dry distillation. Classes of compounds such as carbohydrates, lipids, acids, and esters, that can be correlated with distinct aroma groups, were responsible for the discrimination of samples. However, given the complex nature of the aroma of roasted coffee, it was not possible to assign a specific class of compounds to an exclusive sample group. Both lipids and carbohydrates affected all sample groups. Lipid contribution is attributed to their ability to retain volatiles whereas carbohydrates are precursors of a wide variety of aromatic compounds produced during roasting as a result of Maillard reactions. Nonetheless, regardless of the complexity of the aromatic profile of the coffee samples, all developed models presented high values of sensitivity and specificity, confirming the potential of DRIFTS in the discrimination of roasted coffees according to sensory profiles.

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